

What is claimed is:

(Claim 1)

A method of spectrum analysis in two-dimensional representation wherein as for the specific analyzed object, when spectral data where the intensity of the signal output of a spectrophotometer is represented as a function of its wavenumber, wavelength or time are prepared letting n and m ($n \neq m$) be a positive integer, the n -th and m -th derivatives with respect to wavenumber, wavelength or time of intensity on the spectral profile on the said spectral data are calculated, points on the two-dimensional coordinate plane as the X-Y coordinate system whose X-coordinate is the said n -th derivatives and whose Y-coordinate is the said m -th derivatives, respectively, on the said two-dimensional coordinate plane are plotted, and a two-dimensional derivative plot on the said spectral data is prepared, the specific characteristic information on the said spectral data are obtained based on the said two-dimensional derivative plot and wherein based on the said characteristic information, at least one component band is estimated after the band parameter values regarding at least one component band among the component bands contained in the spectral profile of the analyzed object are estimated, the two-dimensional derivative plot with a specific component band removed is obtained by clearing a specific component band or specific component bands

already estimated or the two-dimensional derivative plot from the spectral profile or a two-dimensional derivative plot of the analyzed object, specific characteristic information based on the two-dimensional derivative plot with this specific component removed is obtained, band parameter values on remaining component bands are estimated based on the said characteristic information, and the estimation of at least one of the other component bands is iterated, component bands are estimated in order, thereby estimating the component band which comprises a spectral profile of the analyzed object.

(Claim 2) A method of spectrum analysis in two-dimensional representation as set forth in claim 1, wherein the component band is a Gaussian band, a Lorentzian band, or a mixture thereof.

(Claim 3) A method of spectrum analysis in two-dimensional representation as set forth in claim 1 or 2, wherein n is 1 and/or 3 and m is n+1.

(Claim 4) A method of spectrum analysis in two-dimensional representation as set forth in claim 2 or 3 wherein in the two-dimensional derivative plot where pairs of the first and second derivatives are represented in X-Y coordinate system, when a typical local minimum indicates the existence of a corresponding component band, an X position of the said local

minimum is a first approximation of band center position X_c of the said component band, setting several points on the said two-dimensional derivative plot in the vicinity of P_a , point of intersection of the said two-dimensional derivative plot with the X -axis, as candidates for the inflection point of the said component band, estimating the bandwidth of the said component band from the candidate of the said inflection point by the following Equation (1), estimating the peak height of the said component band from the distances between the said local minimum and the point(s) of intersection of vertical line passing through the said local minimum and the horizontal line(s) passing through the said candidate points, obtaining the candidates for band parameter values of the said component band, and further obtaining the constraint conditions subjected to the band parameter values for the said component band from the said two dimensional derivative plot, the relation between the bandwidth b_w and the X -position of the inflection point X_p of a single band can be preferably expressed by

$$b_w = (1/K_p) |X_c - X_p| \quad (1)$$

(In Equation, b_w is an estimated value of the bandwidth of a Gaussian or a Lorentzian band, where the coefficient K_p is 0.42466 for Gaussian and 0.288675 for Lorentzian.)

(Claim 5) A method of spectrum analysis in two-dimensional representation as set forth in claim 2 or 3, wherein in the

two-dimensional derivative plot where pairs of the third and fourth derivatives are represented in X-Y coordinate system, when a typical local maximum indicates the existence of a corresponding component band, an X position of the said local maximum is a first approximation of band center position X_c of the said component band, setting several points on the said two-dimensional derivative plot in the vicinity of Q_d , point of intersection of the said two-dimensional derivative plot with the X-axis, as candidates for the secondary inflection point of the said component band, estimating the bandwidth of the said component band from the candidate of the said secondary inflection point by the following Equation (2), estimating the peak height of the said component band from the distances between the said local maximum and the point(s) of intersection of vertical line passing through the said local maximum and the horizontal line(s) passing through the said candidate points, obtaining the candidates for band parameter values of the said component band, and further obtaining the constraint conditions subjected to the band parameter values for the said component band from the said two dimensional derivative plot, the relation between the bandwidth b_w and the X-position of the secondary inflection point X_0 of a single band can be preferably expressed by

$$b_w = (1/K_p) |X_c - X_0| \quad (2)$$

(In the Equation, b_w is an estimated value of the bandwidth

of a Gaussian or a Lorentzian band, where the coefficient K_0 is 0.31508 for Gaussian and 0.16426 for Lorentzian.)

(Claim 6) A method of spectrum analysis in two-dimensional representation as set forth in any one of the claims 1 to 5, wherein the already estimated band parameter values are so adjusted that the already estimated specific component band and the complementary estimation component band with all the estimated component band removed except the said estimated specific component band from a spectral profile or two-dimensional derivative plot of the analyzed object coincide with each other.

(Claim 7) A method of spectrum analysis in two-dimensional representation as set forth in any one of the claims 1 to 6, wherein spectral data are infrared spectra, visible light spectra, ultraviolet spectra, Raman spectra, X-ray diffractograms, chromatograms, etc.